AR201-13901B



**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY



## Alga Toxicity

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline*:** | Other: ECOSAR Computer Model |
| **Year (guideline):** | 1999 |
| **Type (test type):** | Green Alga Toxicity Calculation; EC50 |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Species:** | Freshwater Green Alga (calculated toxicity values are not species specific) |
| **Analytical Monitoring:** | Not applicable |
| **Exposure Period:** | 96 hours |
| **Statistical Method: (FT - ME)*** | Not applicable |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).<br><br>The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of toxicity data for component chemicals is an estimate of the potential toxicity of category products. |

| Chemical | Calculated log $K_{ow}$ | Measured* log $K_{ow}$ |
|---|---|---|
| Isobutane | 2.23 | 2.76 |
| n-butane | 2.31 | 2.89 |
| isobutylene | 2.23 | 2.34 |
| cis-butene-2 | 2.09 | 2.31 |
| trans-butene-2 | 2.09 | 2.33 |
| butene-1 | 2.17 | 2.40 |
| 1,3-butadiene | 2.03 | 1.99 |

* Experimental $K_{ow}$ values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

organic compounds with reliably measured values..

Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.

The seven chemicals selected to represent the alga toxicity range of this category are C4 hydrocarbons that are common across the 12 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (3).

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
3. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

**Results: (FT - RS)**

**Units/Value:**

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Calculated alga toxicity values for 7 chemicals representative of products in the Crude Butadiene C4 Category are as follows:

| Chemical | Calculated log $K_{ow}$ | Alga Toxicity 96-hr EC50 (mg/L) |
|---|---|---|
| Isobutane | 2.23 | 18.06 |
| n-butane | 2.31 | 15.35 |
| isobutylene | 2.23 | 17.44 |
| cis-butene-2 | 2.09 | 23.19 |
| trans-butene-2 | 2.09 | 23.19 |
| butene-1 | 2.17 | 19.71 |
| 1,3-butadiene | 2.03 | 25.27 |

| Chemical | Measured* log $K_{ow}$ | Alga Toxicity 96-hr EC50 (mg/L) |
|---|---|---|
| Isobutane | 2.76 | 6.13 |
| n-butane | 2.89 | 4.71 |
| isobutylene | 2.34 | 13.94 |
| cis-butene-2 | 2.31 | 14.81 |
| trans-butene-2 | 2.33 | 14.22 |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | butene-1 2.40 12.33<br>1,3-butadiene 1.99 27.42<br>* Experimental $K_{ow}$ values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Based on the calculated Kow values, products in this category are expected to have an alga 96-hour EC50 range of 15.35 to 25.27 mg/L. Based on the measured Kow values, products in this category are expected to have an alga 96-hour EC50 range of 4.71 to 27.42 mg/L. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br>The toxicity values are calculated. |
| **Reference: (FT - RE)** | Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "acute toxicity to aquatic plants". Selecting this option refers the reader to information in the "freetext" field for "test substance".
FT - Freetext
IUCLID fields include:
- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Biodegradation

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Other: Technical discussion |
| **Year (guideline):** | Not applicable |
| **Type (test type):** | Not applicable |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Inoculum:** | Not applicable |
| **Exposure Period:** | Not applicable |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | Not applicable |
| **Results: (FT - RS)**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | Not applicable |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| **Conclusion: (FT - CL)** | **Summary**<br><br>In the environment, biodegradation will not contribute significantly to the loss of chemicals in products from the Crude Butadiene C4 category (C4 refers to a chemical with 4 carbons). This category includes three process streams:<br><br>• **C4 Crude Butadiene**<br>• **Butadiene Unit Heavy Ends**<br>• **Full-Range Butadiene Concentrates**<br><br>Twelve CAS numbers (Table 1) identify products derived from these process streams. The products contain various chemicals composed of carbon and hydrogen (Table 2). As discussed below, products in this category are gaseous. If they are released to the environment, their chemical components will partition primarily to the air where they can degrade rapidly by physicochemical reactions. It is far less likely that products from this category will partition to environmental compartments where they could be degraded by bacteria.<br><br>**The Crude Butadiene C4 Category**<br><br>A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Process streams containing 10 to 92% butadiene are referred to as "crude butadiene." With the exception of CAS 106-99-0 (which is pure 1,3-butadiene), the CAS numbers or streams in this category (Table 1) consist of complex mixtures of hydrocarbons (Table 2).<br><br>Most commercial products in this category have a carbon number distribution predominantly between C3 and C5. All of these streams contain significant levels of 1,3-butadiene and olefins, which is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Crude Butadiene C4.<br><br>The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).<br><br>Crude butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the three process streams in this category are: |

- **C4 Crude Butadiene** is produced by the distillation of a condensed portion of cracked gas in an ethylene process. C4 Crude Butadiene typically contains 40% to about 60% 1,3-butadiene, but could contain between 10% and 82% butadiene (Table 2). Other chemicals in this mixed stream are predominately chemicals containing 4 carbons.

- **Butadiene Unit Heavy Ends** is produced by extractive distillation of cracked gas. The 1,3-butadiene content of this mixed stream ranges from 13% to 92% (Table 2). Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. Only three companies report isolating this stream which is more typically an un-isolated intermediate.

- **Full-Range Butadiene Concentrates** is produced from cracked gas after the removal of ethylene or ethylene and propylene. The 1,3-butadiene content of full range butadiene concentrates has been reported to range from 12% to 42% (Table 2). Other chemicals in this mixed stream are those containing three to twelve or more carbons. These streams are intermediates that are not normally isolated in the ethylene process and have been reported as isolated only in infrequent situations.

**Biodegradation of Hydrocarbons**

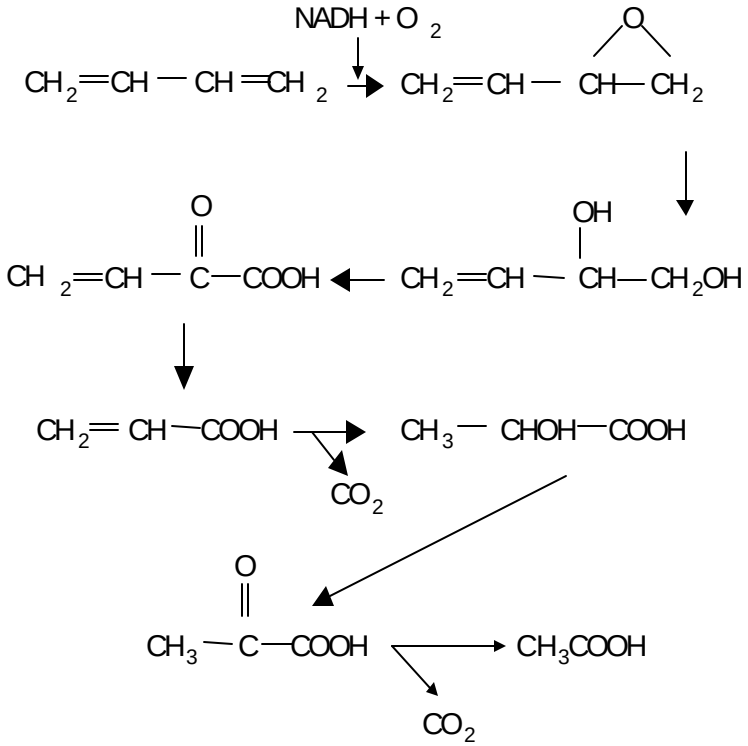
Biodegradation is the use of a chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which can be converted to inorganic forms such as carbon dioxide, nitrate, sulfate, and water.

Products in the Crude Butadiene C4 category are gaseous hydrocarbons, composed predominantly of chemicals with carbon numbers smaller than C5. However, the *Full-Range Butadiene Concentrates* process stream from this category, can contain hydrocarbons greater than C4. These chemicals when isolated individually are not gaseous, but relatively volatile liquids under most environmental conditions.

Several hydrocarbons as well as products that are mixtures of hydrocarbons with carbon numbers greater than C4 have been shown to biodegrade. If released to the environment, biodegradation of these chemicals will occur primarily in aquatic and terrestrial habitats. There is sufficient biodegradation data on hydrocarbons in this category that are greater than C4 to show that these chemicals have a potential to biodegrade to a great extent and not persist in the environment (see the *C5 Noncyclics, Low Benzene Naphtha, and High Benzene Naphtha* HPV Chemical Program test plans from the Olefins Panel of the American Chemistry Council, for specific data and a more detailed discussion of the biodegradability of selected hydrocarbons greater than C4.) The larger proportion of chemicals from this category are gaseous. Consequently, their availability to microbial degraders will be significantly limited.

Component chemicals from all three process streams in this category are simple hydrocarbons (Table 2), the majority of which will partition primarily to the air where physical processes will contribute to their degradation [see the atmospheric oxidation potential (AOP) data (as mediated by hydroxyl radical attack) for specific degradation rates of selected chemicals from this category; AOP data were developed for this category under the HPV Chemical Program]. All chemicals from this category that partition to the air are calculated to degrade rapidly due to physical processes and not persist. Because of the partitioning behavior of chemicals in this category, biodegradative processes will be less likely to contribute to their loss from the environment.

Products from the Crude Butadiene C4 category do not lend themselves to being evaluated for biodegradability using standard experimental techniques because of their physical state. However, there is microbial metabolism information for one of the major chemicals, 1,3-butadiene, in this category that demonstrates that it can be biodegraded. Experimental studies to determine a catabolic pathway for 1,3-butadiene as mediated by a *Nocardia* sp. (3) resulted in the following proposed series of reactions:




The intermediary metabolic steps depicted above result in the production of acetic acid, CH3COOH, which can be further metabolized. In addition, 1,3-butadiene has been estimated to have an aerobic aquatic biodegradation half-life ranging from 1 to 4 weeks (2).

| | |
|---|---|
| | The potential biodegradability of some of the higher molecular weight components including benzene, toluene, xylene, ethylbenzene, and naphthalene has been summarized and metabolic pathways leading to their biodegradation have been described (4). These compounds have been shown to biodegrade to high extents such that if they were to partition to either a terrestrial or aqueous environment, they would be subject to biodegradative processes that would result in their removal from the environment.<br><br>In summary, because the C4 and lighter chemical components of this category will partition to the air, physical degradative processes will dominate their fate. Data show that these chemicals are subject to rapid physical degradation. Chemical components of this category that are greater than C4 also have a potential to partition to the air to a great extent, where they will also degrade rapidly in a similar manner. However, they also have a potential to partition to aquatic and terrestrial environments where they are subject to biological processes that can result in their rapid biodegradation. Overall, products from this category and their component chemicals are expected to degrade rapidly in the environment and not persist.<br><br>**References**<br><br>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA.<br>2. Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. Handbook of Environmental Degradation Rates. H.T. Printup Ed. Lewis Publishers, Chelsea, MI, USA.<br>3. Watkinson, R.J. and H.J. Somerville. 1976. The Microbial Utilization of Butadiene. Shell Research Limited, Sittingbourne Research Centre, Kent, UK.<br>4. van Agteren, M.H., S. Keuning, and D.B. Janssen. 1998. Handbook on Biodegradation and Biological Treatment of Hazardous Organic Compounds. Kluwer Academic Publishers. Boston, CT, USA. |
| **Reliability: (FT - RL)** | Not applicable |
| **Reference: (FT - RE)** | American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Crude Butadiene C4 Category. Rosslyn, VA, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "biodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

FT - Freetext
IUCLID fields include:
- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Boiling Point

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04 |
| **Year (guideline):** | 1999 |
| **Type (test type):** | Not applicable |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Estimation Pressure:** | 760 mm Hg |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | Boiling Point estimations performed by MPBPWIN are based on the calculation method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. **34**: 581-587. |
| **Results: (FT - RS)**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | Chemical / Calculated BP (°C) / Measured* BP (°C)<br>Isobutane 3.21 -11.7<br>n-butane 19.58 -0.5<br>isobutylene 10.18 -6.9<br>cis-butene-2 27.82 0.8<br>trans-butene-2 27.82 0.8<br>butene-1 17.57 -1.3<br>1,3-butadiene 15.55 -4.4<br>* Experimental values are supplied by the MPBPWIN program database (EXP_MBVP.DB) which contains more than 11,000 organic compounds with reliably measured values which are taken from SRC's PHYSPROP Database.<br>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.<br>The seven chemicals selected to represent the boiling range of this category are C4 hydrocarbons that are common across the 12 CAS numbers. Crude butadiene category products arise from |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).<br><br>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Based on the calculated values, products in this category can have a boiling range of 3.21 to 27.82 °C. Based on the measured values, products in this category can have a boiling range of -11.7 to 0.8°C. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br>The results include calculated values based on the chemical structure and experimental values available in the MPBPWIN program and represent a potential boiling point range for products with the 12 CAS numbers listed under test substance. |
| **Reference: (FT - RE)** | Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "boiling point". Selecting this option refers the reader to information in the "freetext" field for "test substance".
FT - Freetext
IUCLID fields include:

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Daphnid Acute Toxicity

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline*:** | Other: ECOSAR Computer Model |
| **Year (guideline):** | 1999 |
| **Type (test type):** | Acute Daphnid Toxicity Calculation; LC50 |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Species:** | Daphnid (calculated toxicity values are not species specific) |
| **Analytical Monitoring:** | Not applicable |
| **Exposure Period:** | 48 hours |
| **Statistical Method: (FT - ME)*** | Not applicable |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).<br><br>The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of toxicity data for component chemicals is an estimate of the potential toxicity of category products.<br><br>Chemical — Calculated log $K_{ow}$ — Measured* log $K_{ow}$<br>Isobutane: 2.23 — 2.76<br>n-butane: 2.31 — 2.89<br>isobutylene: 2.23 — 2.34<br>cis-butene-2: 2.09 — 2.31<br>trans-butene-2: 2.09 — 2.33<br>butene-1: 2.17 — 2.40<br>1,3-butadiene: 2.03 — 1.99<br><br>* Experimental $K_{ow}$ values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.. |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.

The seven chemicals selected to represent the daphnid acute toxicity range of this category are C4 hydrocarbons that are common across the 12 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (3).


1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
3. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.


**Results: (FT - RS)**

**Units/Value:**

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Calculated daphnid acute toxicity values for 7 chemicals representative of products in the Crude Butadiene C4 Category are as follows:

| Chemical | Calculated log $K_{ow}$ | Daphnid Acute 48-hr LC50 (mg/L) |
|---|---|---|
| Isobutane | 2.23 | 28.51 |
| n-butane | 2.31 | 24.11 |
| isobutylene | 2.23 | 27.53 |
| cis-butene-2 | 2.09 | 36.91 |
| trans-butene-2 | 2.09 | 36.91 |
| butene-1 | 2.17 | 31.21 |
| 1,3-butadiene | 2.03 | 40.27 |

| Chemical | Measured* log $K_{ow}$ | Daphnid Acute 48-hr LC50 (mg/L) |
|---|---|---|
| Isobutane | 2.76 | 9.39 |
| n-butane | 2.89 | 7.15 |
| isobutylene | 2.34 | 21.86 |
| cis-butene-2 | 2.31 | 23.28 |
| trans-butene-2 | 2.33 | 22.32 |
| butene-1 | 2.40 | 19.28 |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | 1,3-butadiene 1.99 43.88<br><br>* Experimental $K_{ow}$ values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Based on the calculated Kow values, products in this category are expected to have a daphnid 48-hour LC50 range of 24.11 to 40.27 mg/L. Based on the measured Kow values, products in this category are expected to have a daphnid 48-hour LC50 range of 7.15 to 43.88 mg/L. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br>The toxicity values are calculated. |
| **Reference: (FT - RE)** | Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for " acute toxicity to aquatic invertebrates ". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Fish Acute Toxicity

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline*:** | Other: ECOSAR Computer Model |
| **Year (guideline):** | 1999 |
| **Type (test type):** | Acute Fish Toxicity Calculation; LC50 |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Species:** | Freshwater Fish (calculated toxicity values are not species specific) |
| **Analytical Monitoring:** | Not applicable |
| **Exposure Period:** | 96 hours |
| **Statistical Method: (FT - ME)*** | Not applicable |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.** | Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).<br><br>The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of toxicity data for component chemicals is an estimate of the potential toxicity of category products.<br><br>Chemical — Calculated log $K_{ow}$ — Measured* log $K_{ow}$<br>Isobutane: 2.23 — 2.76<br>n-butane: 2.31 — 2.89<br>isobutylene: 2.23 — 2.34<br>cis-butene-2: 2.09 — 2.31<br>trans-butene-2: 2.09 — 2.33<br>butene-1: 2.17 — 2.40<br>1,3-butadiene: 2.03 — 1.99<br><br>* Experimental $K_{ow}$ values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 |

organic compounds with reliably measured values..

Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.

The seven chemicals selected to represent the fish acute toxicity range of this category are C4 hydrocarbons that are common across the 12 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (3).

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
3. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

**Results: (FT - RS)**

**Units/Value:**

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Calculated fish acute toxicity values for 7 chemicals representative of products in the Crude Butadiene C4 Category are as follows:

| Chemical | Calculated log $K_{ow}$ | Fish Acute 96-hr LC50 (mg/L) |
|---|---|---|
| Isobutane | 2.23 | 26.19 |
| n-butane | 2.31 | 22.03 |
| isobutylene | 2.23 | 25.28 |
| cis-butene-2 | 2.09 | 34.23 |
| trans-butene-2 | 2.09 | 34.23 |
| butene-1 | 2.17 | 28.79 |
| 1,3-butadiene | 2.03 | 37.59 |

| Chemical | Measured* log $K_{ow}$ | Fish Acute 96-hr LC50 (mg/L) |
|---|---|---|
| Isobutane | 2.76 | 8.32 |
| n-butane | 2.89 | 6.28 |
| isobutylene | 2.34 | 19.93 |
| cis-butene-2 | 2.31 | 21.26 |
| trans-butene-2 | 2.33 | 20.36 |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | butene-1 2.40 17.50<br>1,3-butadiene 1.99 40.98<br><br>* Experimental $K_{ow}$ values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Based on the calculated Kow values, products in this category are expected to have a fish 96-hour LC50 range of 22.03 to 37.59 mg/L. Based on the measured Kow values, products in this category are expected to have a fish 96-hour LC50 range of 6.28 to 40.98 mg/L. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br>The toxicity values are calculated. |
| **Reference: (FT - RE)** | Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for " acute toxicity to fish ". Selecting this option refers the reader to information in the "free text" field for "test substance".
FT - Free text
IUCLID fields include:
- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

**Calculated Fish Acute Toxicity**

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Hydrolysis (Stability in Water)

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Other: Technical discussion |
| **Year (guideline):** | Not applicable |
| **Type (test type):** | Not applicable |
| **GLP (Y/N):** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Analytical Monitoring:** | Not applicable |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol** | Not applicable |
| **Results: (FT - RS)**<br>**Units/Value:**<br>• **Note: Analytical method, observations, half-lives by pH, degradation products** | Not applicable |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| **Conclusion: (FT - CL)** | **Summary**<br><br>In the environment, hydrolysis will not contribute to the degradation of chemicals in the Crude Butadiene C4 category (C4 refers to a chemical with 4 carbons). This category includes three process streams:<br><br>• **C4 Crude Butadiene**<br>• **Butadiene Unit Heavy Ends**<br>• **Full-Range Butadiene Concentrates**<br><br>Twelve CAS numbers identify products derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur.<br><br>**The Crude Butadiene C4 Category**<br><br>A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Process streams containing 10 to 92% butadiene are referred to as "crude butadiene." With the exception of CAS 106-99-0 (which is pure 1,3-butadiene), the CAS numbers or streams in this category consist of complex mixtures of hydrocarbons.<br><br>Most commercial products in this category have a carbon number distribution predominantly between C3 and C5. All of these streams contain significant levels of 1,3-butadiene and olefins, which is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Crude Butadiene C4.<br><br>The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).<br><br>Crude butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the three process streams in this category are:<br><br>• **C4 Crude Butadiene** is produced by the distillation of a condensed portion of cracked gas in an ethylene process. C4 Crude Butadiene typically contains 40% to about 60% 1,3-butadiene, but could contain between 10% and 82% butadiene. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. |

- **Butadiene Unit Heavy Ends** is produced by extractive distillation of cracked gas. The 1,3-butadiene content of this mixed stream ranges from 13% to 92%. Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. Only three companies report isolating this stream which is more typically an un-isolated intermediate.

- **Full-Range Butadiene Concentrates** is produced from cracked gas after the removal of ethylene or ethylene and propylene. The 1,3-butadiene content of full range butadiene concentrates has been reported to range from 12% to 42%. Other chemicals in this mixed stream are those containing three to twelve or more carbons. These streams are intermediates that are not normally isolated in the ethylene process and have been reported as isolated only in infrequent situations.

**Hydrolysis of Hydrocarbons as a Function of Molecular Structure**

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water ($H_2O$) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (2,3). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (3) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Crude Butadiene C4 category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3).

Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4). The chemicals in this category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Crude Butadiene C4 category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | **References**<br><br>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.<br>2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.<br>3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.<br>4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA. |
| **Reliability: (FT - RL)** | Not applicable |
| **Reference: (FT - RE)** | American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Crude Butadiene C4 Category. Rosslyn, VA, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "hydrolysis". Selecting this option refers the reader to information in the "freetext" field for "test substance".
FT - Freetext
IUCLID fields include:
RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Melting Point

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04 |
| **Year (guideline):** | 1999 |
| **Type (test type):** | Not applicable |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle.<br><br>Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.<br><br>The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. |
| **Results: (FT - RS)**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | Chemical / Calculated MP (°C) / Measured* MP (°C)<br>Isobutane: -132.55 / -138.3<br>n-butane: -120.28 / -138.2<br>isobutylene: -130.88 / -140.4<br>cis-butene-2: -120.41 / -105.5<br>trans-butene-2: -120.41 / -105.5<br>butene-1: -121.74 / -145.0<br>1,3-butadiene: -123.21 / -108.9<br><br>* Experimental values are supplied by the MPBPWIN program database (EXP_MBVP.DB) which contains more than 11,000 organic compounds with reliably measured values which are taken from SRC's PHYSPROP Database.<br><br>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | Program, and designated Crude Butadiene C4.<br><br>The seven chemicals selected to represent the melting range of this category are C4 hydrocarbons that are common across the 12 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).<br><br>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Based on the calculated values, products in this category can have a melting range of -132.55 to -120.28 °C. Based on the measured values, products in this category can have a melting range of -145.0 to -105.5°C. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br><br>The results include calculated values based on the chemical structure and experimental values available in the MPBPWIN program and represent a potential melting range for products with the 12 CAS numbers listed under test substance. |
| **Reference: (FT - RE)** | Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "melting point". Selecting this option refers the reader to information in the "freetext" field for "test substance".

FT - Freetext

IUCLID fields include:

- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Partition Coefficient

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04 |
| **Year (guideline):** | 1999 |
| **Type (test type):** | Not applicable |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Estimation Temperature:** | 25°C |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. *J. Pharm. Sci*. **84**:83-92. |
| **Results: (FT - RS)**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | Chemical / Calculated log $K_{ow}$ / Measured* log $K_{ow}$<br>Isobutane: 2.23 / 2.76<br>n-butane: 2.31 / 2.89<br>isobutylene: 2.23 / 2.34<br>cis-butene-2: 2.09 / 2.31<br>trans-butene-2: 2.09 / 2.33<br>butene-1: 2.17 / 2.40<br>1,3-butadiene: 2.03 / 1.99<br><br>* Experimental $K_{ow}$ values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.<br><br>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.<br><br>The seven chemicals selected to represent the partition coefficient range of this category are C4 hydrocarbons that are common across the 12 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).<br><br>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Based on the calculated $K_{ow}$ values, products in this category can have a partition coefficient range of 2.03 to 2.31. Based on the measured $K_{ow}$ values, products in this category can have a partition coefficient range of 1.99 to 2.89. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br><br>The results include calculated values based on the chemical structure and experimental values available in the KOWWIN program and represent a potential partition coefficient range for products with the 12 CAS numbers listed under test substance. |
| **Reference: (FT - RE)** | Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "partition coefficient". Selecting this option refers the reader to information in the "freetext" field for "test substance".
FT - Freetext
IUCLID fields include:
RL - Reliability

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Photodegradation (Direct)

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Other: Technical discussion |
| **Year (guideline):** | Not applicable |
| **GLP (Y/N):** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Type (air, soil, water, other):** | Not applicable |
| **Light Source:** | Not applicable |
| **Light Spectrum:**<br>• **Wave length value (upper/lower)** | Not applicable |
| **Relative Intensity:** | Not applicable |
| **Test Substance Spectrum:** | Not applicable |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol** | Not applicable |
| **Direct Photolysis**:**<br>**Results: half-life, % degradation, quantum yield** | **Summary**<br><br>In the environment, photolysis will not significantly contribute to the degradation of chemicals in the Crude Butadiene C4 category (C4 refers to a chemical with 4 carbons). The Crude Butadiene C4 category includes three process streams:<br><br>• **C4 Crude Butadiene**<br>• **Butadiene Unit Heavy Ends**<br>• **Full-Range Butadiene Concentrates**<br><br>Twelve CAS numbers (Table 1) identify products derived from these process streams. As discussed below, the reaction process involved in direct photolysis occurs when sufficient light energy excites a molecule to the degree that a structural transformation occurs. In general, products in this category do not contain component chemicals (Table 2) that will undergo direct photolysis.<br><br>**The Crude Butadiene C4 Category** |

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. Process streams containing 10 to 92% butadiene are referred to as "crude butadiene." With the exception of CAS 106-99-0 (which is pure 1,3-butadiene), the CAS numbers or streams in this category (Table 1) consist of complex mixtures of hydrocarbons (Table 2).

Most commercial products in this category have a carbon number distribution predominantly between C3 and C5. All of these streams contain significant levels of 1,3-butadiene and olefins, which is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Crude Butadiene C4.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

Crude butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the three process streams in this category are:

- **C4 Crude Butadiene** is produced by the distillation of a condensed portion of cracked gas in an ethylene process. C4 Crude Butadiene typically contains 40% to about 60% 1,3-butadiene, but could contain between 10% and 82% butadiene (Table 2). Other chemicals in this mixed stream are predominately chemicals containing 4 carbons.

- **Butadiene Unit Heavy Ends** is produced by extractive distillation of cracked gas. The 1,3-butadiene content of this mixed stream ranges from 13% to 92% (Table 2). Other chemicals in this mixed stream are predominately chemicals containing 4 carbons. Only three companies report isolating this stream which is more typically an un-isolated intermediate.

- **Full-Range Butadiene Concentrates** is produced from cracked gas after the removal of ethylene or ethylene and propylene. The 1,3-butadiene content of full range butadiene concentrates has been reported to range from 12% to 42% (Table 2). Other chemicals in this mixed stream are those containing three to twelve or more carbons. These streams are intermediates that are not normally isolated in the ethylene process and have been reported as isolated only in infrequent situations.

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

**Photolysis of Hydrocarbons**

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (2). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (2). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (2). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima ($\lambda_{max}$) and associated molar absorptivities ($\varepsilon$) for selected unsaturated hydrocarbons are shown below (2):

**Direct Photolysis**: (continued)**

**Results: half-life, % degradation, quantum yield**

| Hydrocarbon | l **below 290 nm** | | l **above 290 nm** | |
|---|---|---|---|---|
| | $l_{max}$ | e | $l_{max}$ | e |
| **Ethylene** | 193 | 10,000 | | |
| 1,3-Butadiene | 217 | 2,090 | | |
| Benzene | 255 | 215 | | |
| Naphthalene | 221<br>270 | 100,000<br>5,000 | 311 | 250 |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | Olefins with one double bond, two conjugated double bonds, or multiple un-conjugated bonds, which constitute the majority of the chemicals in the Crude Butadiene C4 category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2).<br><br>Single ring aromatics also do not absorb sufficient light energy above 290 nm to cause photolysis. However, fused aromatic ring systems such as naphthalene and PAHs absorb sufficient light energy above 290 to potentially result in photolysis (2). Except for naphthalene, which has been identified in one of the three process streams, products in this category do not contain component molecules of significant concentration (>2% by weight) that will undergo direct photolysis. Naphthalene irradiated at 313 nm has a quantum yield for photolysis of 0.015 and a half-life of 70 hours (4).<br><br>In general, most products in the Crude Butadiene C4 category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.<br><br>**References**<br><br>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA.<br>2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.<br>3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.<br>4. Zepp, R. G and P. F. Schlotzhauer. Photoreactivity of Selected Aromatic Hydrocarbons in Water, in Polynuclear Aromatic Hydrocarbons. P. W. Jones and P. Leber, eds., Ann Arbor Science Publishers, Inc., Ann Arbor, MI, USA. pp. 141-158. |
| **Indirect Photolysis**:**<br>• **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life** | Not applicable |
| **Degradation Products**:**<br>• **Note: Identification,** | Unknown |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| **concentration** | |
|---|---|
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Not applicable |
| **Reliability: (FT - RL)** | Not applicable |
| **Reference: (FT - RE)** | American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Crude Butadiene C4 Category. Rosslyn, VA, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "photodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".
** In IUCLID, provide addtional discussion if needed in the results freetext
FT - Freetext
IUCLID fields include:
- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Photodegradation (Indirect)

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04 |
| **Year (guideline):** | 1999 |
| **GLP (Y/N):** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Type (air, soil, water, other):** | Not applicable |
| **Light Source:** | Sunlight |
| **Light Spectrum:**<br>• **Wave length value (upper/lower)** | Natural sunlight |
| **Relative Intensity:** | 1 |
| **Test Substance Spectrum:** | Not applicable |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol** | Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.<br><br>Temperature: 25°C<br>Sensitizer: OH radical<br>Concentration of Sensitizer: 1.5 $E^6$ OH radicals/$cm^3$ |
| **Direct Photolysis**:**<br>**Results: half-life, % degradation, quantum yield** | Not applicable |
| **Indirect Photolysis**:**<br>• **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life** | In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (1,2). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (3).<br><br>AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric |

concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

| Chemical | Calculated* half-life (hrs) | OH- Rate Constant ($cm^3$/molecule-sec) |
|---|---|---|
| Isobutane | 52.6 | $2.4\ E^{-12}$ |
| n-butane | 48.8 | $2.6\ E^{-12}$ |
| isobutylene | 2.5 | $51.7\ E^{-12}$ |
| cis-butene-2 | 2.3 | $56.7\ E^{-12}$ |
| trans-butene-2 | 2.0 | $64.3\ E^{-12}$ |
| butene-1 | 4.7 | $27.4\ E^{-12}$ |
| 1,3-butadiene | 1.9 | $66.6\ E^{-12}$ |

* Atmospheric half-life values are based on a 12-hr day.

Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.

The seven chemicals selected to represent the atmospheric half-life range of this category are C4 hydrocarbons that are common across the 12 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (4).

References:

1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem*. **7**:435-442.
2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.
3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299.
4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

| | |
|---|---|
| **Degradation Products**:** | Unknown |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| • **Note: Identification, concentration** | |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Atmospheric oxidation vial hydroxyl radical can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 1.9 to 52.6 hours as a result of indirect photolysis by hydroxyl radical attack. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br>The results include values calculated using the AOPWIN program and represent a potential atmospheric half-life range for products with the 12 CAS numbers listed under test substance. |
| **Reference: (FT - RE)** | Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "photodegradation". Selecting this option refers the reader to information in the "freetext" field for "test substance".
** In IUCLID, provide additional discussion if needed in the results freetext
FT - Freetext
IUCLID fields include:
RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
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**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Transport / Distribution (Fugacity)

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Calculated according to Mackay Level I, EQC Model version 1.01 |
| **Year (guideline):** | 1997 |
| **Type (test type):** | Not applicable |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Estimation Temperature:** | 25°C |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.<br><br>Physical properties input into the model are those calculated by the EPIWIN Estimation v 3.04 program (1) or supplied by the databases of experimental values contained with EPIWIN. Output data from the equilibrium model provides basic information on the potential distribution of chemicals between selected environmental compartments (i.e. air, water, soil, sediment, suspended sediment, biota).<br><br>1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. |
| **Results: (FT - RS)**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | The following chemicals are representative of products in the Crude Butadiene C4 Category, which are complex, multi-constituent substances. The range of partitioning data for component chemicals is an estimate of the partitioning behavior for category products. |

| | Calculated* Percent Distribution | | Measured** Percent Distribution | |
|---|---|---|---|---|
| Chemical | Air | Water | Air | Water |
| Isobutane | 99.99 | 0.01 | 99.99 | 0.01 |
| n-butane | 99.98 | 0.02 | 99.99 | 0.01 |
| isobutylene | 99.98 | 0.02 | 99.99 | 0.01 |
| cis-butene-2 | 99.97 | 0.03 | 99.98 | 0.02 |
| trans-butene-2 | 99.97 | 0.03 | 99.98 | 0.02 |
| butene-1 | 99.98 | 0.02 | 99.99 | 0.01 |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | 1,3-butadiene 99.97 0.03 99.97 0.03<br><br>* Distribution values determined using input data calculated by the EPIWIN program<br>**Distribution values determined using input data supplied by the EPIWIN program experimental databases (EXPKOW.DB, EXP_MBVP.DB, and EXP_MBVP.DB) which contain more than 11,000 organic compounds with reliably measured values.<br><br>Distribution of each chemical to each remaining compartment (soil, sediment, suspended sediment, biota) was calculated as less than 0.01%. Mobility in the environment is expected to be high due to the relatively high water solubility and high vapor pressure of these chemicals.<br><br>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.<br><br>The seven chemicals selected to represent the transport / distribution range of this category are C4 hydrocarbons that are common across the 12 CAS numbers and can represent a significant proportion of a product. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).<br><br>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| **Conclusion: (FT - CL)** | Products in the Crude Butadiene C4 Category are expected to distribute to air with a small percentage partitioning to water. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br>The input data used to run the EQC Level I model include estimated values calculated by the EPIWIN program based on chemical structure, and experimental values supplied by the EPIWIN program databases. The partitioning data represent a potential distribution range for products with the 12 CAS numbers listed under test substance. Computer modeling is an accepted method of assessing environmental distribution of chemicals. |
| **Reference: (FT - RE)** | Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "transport / distribution". Selecting this option refers the reader to information in the "free text" field for "test substance".
FT - Free text
IUCLID fields include:
- RL - Reliability
- TC - Test Conditions
- RE - Reference
- RS - Results
- TS - Test Substance
- SO - Source
- CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Vapor Pressure

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04 |
| **Year (guideline):** | 1999 |
| **Type (test type):** | Not applicable |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Estimation Temperature:** | 25°C |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | Vapor Pressure estimations performed by MPBPWIN are based on the average result of the calculation methods of Antoine and Grain. Both methods use boiling point for the calculation.<br><br>The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990.<br><br>A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985. |
| **Results: (FT - RS)**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | Chemical / Calculated VP (hPa) / Measured* VP (hPa)<br>Isobutane: 3.45 $E^3$ / 3.08 $E^3$<br>n-butane: 2.41 $E^3$ / 2.43 $E^3$<br>isobutylene: 2.97 $E^3$ / 3.08 $E^3$<br>cis-butene-2: 2.31 $E^3$ / 2.33 $E^3$<br>trans-butene-2: 2.31 $E^3$ / 2.33 $E^3$<br>butene-1: 2.48 $E^3$ / 3.00 $E^3$<br>1,3-butadiene: 2.73 $E^3$ / 2.81 $E^3$<br><br>* Experimental values are supplied by the MPBPWIN program database (EXP_MBVP.DB) which contains more than 11,000 organic compounds with reliably measured values which are taken from SRC's PHYSPROP Database.<br><br>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a |

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

| | |
|---|---|
| | category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.<br><br>The seven chemicals selected to represent the vapor pressure range of this category are C4 hydrocarbons that are common across the 12 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).<br><br>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Based on the calculated values, products in this category can have a vapor pressure range of 2.31 $E^3$ to 3.45 $E^3$ hPa. Based on the measured values, products in this category can have a vapor pressure range of 2.33 $E^3$ to 3.08 $E^3$ hPa. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br><br>The results include calculated values based on the chemical structure and experimental values available in the MPBPWIN program and represent a potential vapor pressure range for products with the 12 CAS numbers listed under test substance. |
| **Reference: (FT - RE)** | Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

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* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "vapor pressure". Selecting this option refers the reader to information in the "freetext" field for "test substance".
FT - Freetext
IUCLID fields include:
RL - Reliability
TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

# CRUDE BUTADIENE C4 ROBUST SUMMARY

## Water Solubility

| | |
|---|---|
| **Test Substance*:** | Other TS |
| **Method/Guideline:** | Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04 |
| **Year (guideline):** | 1999 |
| **Type (test type):** | Not applicable |
| **GLP:** | Not applicable |
| **Year (study performed):** | Not applicable |
| **Estimation Temperature:** | 25°C |
| **Test Conditions: (FT - TC)**<br>• **Note: Concentration prep., vessel type, replication, test conditions.** | Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". *Environ. Toxicol. Chem.* **15**:100-106. 1995. |
| **Results: (FT - RS)**<br>**Units/Value:**<br>• **Note: Deviations from protocol or guideline, analytical method.** | See table below<br><br>* Experimental $K_{ow}$ values supplied by the WSKOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.<br><br>Commercial products in this category can have a carbon number distribution predominantly between C3 and C5. These products can contain significant levels of 1,3-butadiene and similar low molecular weight olefins, which is why they are considered a category for purposes of the High Production Volume Chemical Program, and designated Crude Butadiene C4.<br><br>The seven chemicals selected to represent the water solubility range of this category are C4 hydrocarbons that are common across the 12 CAS numbers. Crude butadiene category products arise from production processes associated with ethylene |

| Chemical | Calculated WS (mg/L) | Measured* WS (mg/L) |
|---|---|---|
| Isobutane | 496.4 | 175.1 |
| n-butane | 424.1 | 135.6 |
| isobutylene | 495.6 | 399.2 |
| cis-butene-2 | 652.7 | 423.5 |
| trans-butene-2 | 652.7 | 407.1 |
| butene-1 | 557.7 | 354.8 |
| 1,3-butadiene | 732.4 | 792.3 |

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| | |
|---|---|
| | manufacturing. More information on the Crude Butadiene C4 category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).<br><br>1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Crude Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. |
| **Test Substance: (FT - TS)** | 106-99-0 1,3-Butadiene<br>25167-67-3 Butenes<br>68477-41-8 Distillate (Petroleum), Extractive C3-5<br>68955-28-2 Gases, (Petroleum) Light Steam Cracked, Butadiene Concentrate<br>68476-44-8 Hydrocarbons, >C3<br>68512-91-4 Hydrocarbons C3 – C4 Rich Petroleum Distillates<br>68187-60-0 Hydrocarbons, C4, Ethane-Propane Cracked<br>68476-52-8 Hydrocarbons, C4, Ethylene Manufactured By-Product<br>68956-54-7 Hydrocarbons C4, Unsaturated<br>69103-05-5 Hydrocarbons, C4-7, Butadiene Manufactured By-Product<br>64742-83-2 Naphtha, (Petroleum), Light Steam-Cracked<br>68513-68-8 Residues (Petroleum), Deethanizer Tower |
| **Conclusion: (FT - CL)** | Based on the calculated $K_{ow}$ values, products in this category can have a water solubility range of 424.1 to 732.4 mg/L. Based on the measured $K_{ow}$ values, products in this category can have a water solubility range of 135.6 to 792.3 mg/L. |
| **Reliability: (FT - RL)** | (2) Reliable with restrictions<br><br>The results include values estimated using calculated $K_{ow}$ and experimental $K_{ow}$ values available in the WSKOWWIN program and represent a potential water solubility range for products with the 12 CAS numbers listed under test substance. |
| **Reference: (FT - RE)** | Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. |
| **Other (source): (FT - SO)** | American Chemistry Council, Olefins Panel |

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "water solubility". Selecting this option refers the reader to information in the "freetext" field for "test substance".
FT - Freetext
IUCLID fields include:
RL - Reliability

**CAS No.:** 106-99-0; 25167-67-3; 68477-41-8; 68955-28-2; 68476-44-8; 68512-91-4; 68187-60-0; 68476-52-8; 68956-54-7; 69103-05-5; 64742-83-2; 68513-68-8

TC - Test Conditions
RE - Reference
RS - Results
TS - Test Substance
SO - Source
CL - Conclusion